SF 298 MASTER COPY KEEP THIS COPY FOR REPRODUCTION PURPOSES

REPORT DOCUMENTATION PAGE

Form Approved OMB NO. 0704-0188

1. AGENCY USE ONLY *(Leave blank)*

2. REPORT DATE
08/22/1996

3. REPORT TYPE AND DATES COVERED
FINAL, 1 Aug 92 - 28 Feb 96

4. TITLE AND SUBTITLE
Theoretical Study of Quantum Systems Interacting with a Phonon Bath

5. FUNDING NUMBERS
DAAL03-92-G-0368

6. AUTHOR(S)
Walter Poetz

7. PERFORMING ORGANIZATION NAMES(S) AND ADDRESS(ES)
Univ of Illinois at Chicago
Department of Physics
Chicago, Illinois 60680

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)
U.S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709-2211

10. SPONSORING / MONITORING AGENCY REPORT NUMBER
ARO 30582.16-PH

11. SUPPLEMENTARY NOTES
The views, opinions and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy or decision, unless so designated by other documentation.

12a. DISTRIBUTION / AVAILABILITY STATEMENT
Approved for public release; distribution unlimited.

12 b. DISTRIBUTION CODE

19960910 016

13. ABSTRACT *(Maximum 200 words)*

We have developed two complimentary theoretical approaches to study the dynamics of coupled electron–phonon systems. The first is based on coherent–state functional representations of ensemble averages and has been shown useful in the strong coupling limit of the electron–phonon coupling. A new exactly solvable model has been identified. A two–level system coupled to phonons has been used to demonstrate irreversible dynamics. The second approach is based on non–equilibrium Green's functions which were used to derive Boltzmann–Bloch equations useful in the weak coupling limit. It has been used to discuss

(continued on reverse side)

DTIC QUALITY INSPECTED 3

14. SUBJECT TERMS
quantum transport, electron--phonon system, phase breaking, dissipation, double well, mesoscopics, coherence

15. NUMBER IF PAGES
9

16. PRICE CODE

17. SECURITY CLASSIFICATION OR REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UL

NSN 7540-01-280-5500

Standard Form 298 (Rev. 2-89)
Prescribed by ANSI Std. 239-18
298-102

FINAL PROGRESS REPORT

1. ARO PROPOSAL NUMBER: 30582–PH

2. PERIOD COVERED BY REPORT: Aug 1, 1992 – June 30, 1996

3. TITLE OF PROPOSAL: Theoretical Study of Quantum Systems Interacting with a Phonon Bath

4. CONTRACT OR GRANT NUMBER: DAAL03–92–G–0368

5. NAME OF INSTITUTION: University of Illinois at Chicago

6. AUTHORS OF REPORT: Walter Poetz

PROJECT SUMMARY

We have developed two complimentary theoretical approaches to study the dynamics of coupled electron–phonon systems. The first is based on coherent–state functional representations of ensemble averages and has been shown useful in the strong coupling limit of the electron–phonon coupling. A new exactly solvable model has been identified. A two–level system coupled to phonons has been used to demonstrate irreversible dynamics. The second approach is based on non–equilibrium Green's functions which were used to derive Boltzmann–Bloch equations useful in the weak coupling limit. It has been used to discuss screening in such systems and to gain microscopic understanding of phase breaking in semiconductor systems. Specifically, the damping of charge oscillations and THz pulse emission has been studied for GaAs–AlGaAs double wells. Scattering theory has been developed for open mesoscopic electronic devices, formally exact in one dimension and heuristically for higher dimension. The signature of Bloch oscillations in the I–V characteristics of p–i–n diodes has been investigated. Exact open boundary conditions have been developed for the one–dimensional time–dependent Schrödinger equation and applied to a study of the dynamics of multi–barrier semiconductor heterostructures.

TABLE OF CONTENTS

I. PROJECTS ADDRESSED WITHIN THIS GRANT

The main body of work supported by this grant was devoted to a theoretical study of the dynamics of coupled electron–phonon systems out of equilibrium. Two complementary theoretical methods have been developed to accomplish the task of descibing irriversibility and dissipation in this type of quantum system. The motivation for such work was and is a microscopic understanding of phase breaking and structural dephasing in semiconductors on a sub–picosecond time scale. However, the approaches developed here are more general and allow application to other quantum systems, such as interacting spin systems. A coherent–state functional integral approach for (strongly) coupled electron–phonon systems has been presented. It is most suitable for complex electron–phonon systems which may either be described within mean–field approximations or treated exactly. Indeed, we have found a hitherto unknown exact solution to a coupled electron–phonon system. The second approach is based on non–equilibrium Green's functions and diagrammatic expansions. It is useful when the system is structurally relatively simple and dissipative effects are dominated by the electron–electron interaction, however, we have also included the electron–phonon interaction.

Several aspects of ballistic charge transport have been investigated. (i) Scattering theory for multi–dimensional mesoscopic (ballistic) electronic devices (normal metals and/or semiconductors) has been developed heuristically, as well as exactly for quasi–one–dimensional systems. This approach has been applied to the study of Zener tunneling in highly doped n-i-p diodes. (ii) Exact open boundary conditions for the time–dependent Schrödinger equation have been developed. They allow an accurate description of the action of contacts for a large classs of electronic devices.

Finally, at the beginning of this project, the electronic confinement in amorphous semiconductor quantum wells has been investigated. This work was motivated by experimental data which indicated such an effect and potential application of such systems in electronic devices.

II. SUMMARY OF MOST IMPORTANT RESULTS

A. Quantum Transport in Coupled Electron–Hole Systems

(a) An exact formulation of *the dynamics of coupled-electron phonon systems* in terms of coherent–state functional functional integrals in electronic degrees of freedom has been developed. It has been used to derive mean–field solutions which, in turn, have been used to study the irreversibe time–evolution of a two–level system coupled to a phonon bath. Based on this approach, we have identified an *exactly solvable model of a coupled many-fermion-boson system* which can be used to model systems such as multiply charged point defects in solids. Its thermal equilibrium and linear–response properties have been given exactly. This model may either be used to (largely analytically) study general features of real systems, or as a test for approximation schemes. Applicability of this approach to spin systems has been explored.

(b) For systems which cannot be adequately described within mean–field approximations we have derived *generalized Boltzmann-Bloch equations* for coupled electron–phonon multiband systems within the Keldysh approach for nonequilibrium Green's functions. They are generalizations of coherent semiconductor Bloch equations in that they account self–consistently for screened particle interactions. They are numerically attractive because they retain the Markovian character of the simpler Boltzmann equation, yet, account for phase coherence in the system and, by means of interband polarizations, for non–Markovian effects for the carrier distribution function.

Their application to *asymmetric semiconductor double wells* has revealed that the carrier–carrier Coulomb interaction plays an important, if not the predominant, role for the carrier dynamics. Hartree–Fock contributions provide significant (frequency) renormalization, excitonic effects, as well as damping of coherent charge oscillations. Pulsed THz light emission from the system was analyzed theoretically and good agreement with experiment has been found. This study reveals the limitations of tunability of THz radiation from double wells. In particular, phase breaking due to the carrier–carrier interaction has been found to clearly dominate structural dephasing due to the electronic structure of the system. Charge oscillations require a charge density below a few 10^10 electrons per cm^2.

In a coupled electron–phonon system it has been shown that dynamic screening hybridizes the electron–electron and eletron–phonon interactions. Due to a loosening of energy conservation in a time–dependent problem, this hybridization is more pronounced than in equilibrium. The effect of screening on the matrix elements for the particle–particle interactions has been identified at several levels of approximation.

A comparison between the density matrix approach and the nonequilibrium Greens function method (NEGFM) used here revealed that, while both are equivalent, the latter is conceptually simpler to calculate higher–order corrections.

B. Ballistic Transport

(a) In collaboration with the Walter Schottky Institute at the Technical University in Garching, Germany, we have used a full–zone many–band model for Zener tunneling to study the effects of Wannier–Stark (WS) states in the current response of highly doped p–i–n junctions in both bulk and superlattices. Our detailed calculations have lead to the following conclusions: Conventional two–band models can give only a qualitative picture of Zener tunneling whereas our approach gives quantitative agreement with experiment. At least three bands – an emitter band, a collector band and the band that displays the WS ladder – need to be involved to allow detection of WS ladders in the current response. These resonances should be observable not only in superlattices but also in the bulk. However, in bulk GaAs, for example, n and p doping in excess of $10^{18}cm^{-3}$ and a width of the i zone of no more than $\approx 25nm$ are required. Contrary to earlier (analytical) treatments we show that WS states are stable with respect to (small) misalignment of the electric field.

(b) Methods of the theory of ordinary differential equations have been used to explicitly and mathematically rigorously show *orthogonality and completeness* (together with bound states) *of scattering states* in one–dimensional systems with either step–like or periodic asymptotic behavior. This work is of fundamental relevance to the application of linear–response theory to transport in mesoscopic electronic device structures and allows calculation of absolute current densities.

Rigorous conditions on potentials with periodic (crystal) potential asymptotics and constant potential asymptotics have been identified for which a *scattering theory* may be developed in one spatial dimension. A rigorous and general proof of orthogonality and completeness of scattering states (together with bound states) has been given for both cases, which, for instance, cover lateral transport in nearly arbitrary heterostructures. The associated S–matrices are defined and conditions under which the S–matrix is unitary and continuous are established

We have also applied a more general heuristic scattering–theoretical argument to show completeness and orthogonality of scattering states for mesoscopic systems under very general conditions in higher dimensions. In particular, we have identified the (structural) conditions under which *ballistic transport models* (Landauer model) are valid.

(c) *Exact open boundary conditions* for constant potential asymptotics have been developed and implemented into a time–dependent analysis of lateral transport in semiconductor heterostructures based on the Schrödinger equation. This makes possible an efficient self–consistent study of the transient current response of a large class of semiconductor heterostructures. An analysis of the resonant–tunneling (RT) diode has revealed the presence of intrinsically supported current oscillations which are closely related to its intrinsic bistability. The transition from RT behavior of a double barrier to Bloch oscillations in superlattices, is currently under investigation.

C. Electron Confinement in Amorphous Semiconductor Quantum Wells

We have conducted a study of *electron confinement effects in amorphous semiconductor heterostructures.* Existence or absence of confinement gives valuable information on the electronic structure of amorphous semiconductors and their potential for electronic device applications. Our calculations have, for the first time, firmly established that electronic quantum confinement, as reported in some experiments (but not in others) must be expected in narrow a–Si/SiC layers. Effects should be observable at the conduction–band edge in form of step–like features in the density of states. However, our calculations indicate that these effects should be observable only up to layer thicknesses of about 20 Å, thus shedding doubt on the interpretation of earlier experiments on significantly wider wells.

III. LIST OF SCIENTIFIC ARTICLES

(A) SUBMITTED:

W. Pötz, and U. Hohenester, "Dynamic Screening in Nonequilibrium Electron–Phonon Systems", June 1996, to Journal of Physics.

(B) IN PRESS:

M. A. Talebian and W. Pötz, "Time–Dependent Current Response of Semiconductor Multi–Barriers", Superlatt. and Microstruct., accepted, May 1996.(*)
W. Pötz, "Microscopic Theory of Coherent Carrier Dynamics and Phase–Breaking in Semiconductors", accepted in Phys. Rev. B.(*)
M. A. Talebian and W. Pötz, "Open Boundary Conditions for a Time–Dependent Analysis of the Resonant Tunneling Structure", Dec. 18, 1995, accepted in APL.(*)
F. Gesztesy, R. Nowell, and W. Pötz, "One–Dimensional Scattering Theory for Quantum Systems with Nontrivial Spatial Asymptotics", Aug. 1995, submitted to Differential and Integral Equations. (*)

(C) PUBLISHED:

W. Pötz, "Infra–red Light Emission from Semiconductor Double Wells", J. Appl. Phys. Lett. **68**, 2553–2555 (1996).(*)
U. Hohenester and W. Pötz, "Green's Functions Versus Density Matrices: Critical Remarks on Free–Carrier Screening in Highly Excited Semiconductors", in "Hot Carriers in Semiconductors", edited by K. Hess, J. P. Leburton, and U. Ravaioli, p. p. 109–111 (Plenum, New York, 1996).
W. Pötz and U. Hohenester, "Free–Carrier Screening in Coupled Electron–Phonon Systems out of Equilibrium", in "Hot Carriers in Semiconductors", edited by K. Hess, J. P. Leburton, and U. Ravaioli, p. 425–427 (Plenum, New York, 1996).
W. Pötz, M. Žiger and P. Kocevar, "Tunneling of Laser–Generated Free Electrons in Semiconductor Double Wells", Phys. Rev. B **52**, 1959–1969 (1995).(*)
W. Pötz, "Scattering Theory for Mesoscopic Quantum Systems with Non–Trivial Spatial Asymptotics in One Dimension", Oct. 94, J. Math. Phys. **36**, 1707-1740 (1995).(*)
M. Žiger and W. Pötz, "Loss of Phase Coherence in Semiconductor Heterostructures Due to the Coulomb Interaction", Proc. 3^{rd} Int. Workshop on Computational Electronics, Portland, OR, May 17–20, edited by S. M. Goodnick, p. 167–170 (Oregon State University Press, Corvallis, 1994).

Aldo Di Carlo, Peter Vogl, and Walter Pötz, "Theory of Zener Tunneling and Wannier–Stark States in Semiconductors", Phys. Rev. B **50**, 8358–8377 (1994).(*)

Aldo Di Carlo, Walter Pötz, and Peter Vogl, " Scattering Theory of Zener Tunneling and Stark Ladders in Semiconductors", published in "Il Vuoto" (more precice information not available).

M. Žiger, W. Pötz, and P. Kocevar, "Damping of Charge Oscillations in Double–Well Structures by the Coulomb Interaction", in *Ultrafast Phenomena in Semiconductors*, D. K. Ferry and H. van Driel, Editors, Proc. SPIE 2142, 87 (1994).(*)

J. Zhang and W. Pötz, "Exactly Solvable Many–Fermion Independent–Boson Systems", Phys. Rev. B **48**, 11583–11591 (1993).(*)

Z. Q. Li and W. Pötz, "Theoretical Study of Carrier Confinement in a-Si–SiC Quantum Wells, Phys. Rev. B **47**, 6509–6517 (1993).(*)

Z. Q. Li and W. Pötz, "Electronic Density of States of Semiconductor Alloys from Lattice–Mismatched Isovalent Binary Constituents", Phys. Rev. B **46**, 2109–2118 (1992).(*)

W. Pötz and J. Zhang, "Coherent–State Functional Integral Approach to High–Field Transport in Coupled Electron–Phonon Systems", Phys. Rev. B **45**, 11496–11510 (1992). (*)

W. Pötz, "On the Current Response in Semiconductor Heterostructures within the Independent–Electron Picture", J. Appl. Phys. **71**, 2297-2302 (1992).(*)

W. Pötz, "Transport Theory for Coupled Electron–Phonon Systems: An Independent Particle Approach", Superlatt. Microstruct. **11**, 175–178, (1992).(*)

(*) indicates refereed publications.

(D) PhD Thesis:

• Z. Q. Li, "Electronic Structure of Disordered Semiconductors", Ph.D. Thesis, supervised by W. Pötz, University of Illinois at Chicago, June 1993.

• J. Zhang, "Coherent–State Functional Integral Approach to Coupled Fermion–Boson Systems", Ph.D. Thesis, supervised by W. Pötz, University of Illinois at Chicago, Dec. 1993.

IV. LIST OF PARTICIPATING SCIENTIFIC PERSONNEL AND DEGREES AWARDED

W. Pötz (PI, full period)

Z. Q. Li 20 % research assistantship, Aug. 1992 to June 1993), *PhD Graduation* in June of 1993.

J. Zhang (50% , Aug. 1992 to Dec. 1993), *PhD Graduation* in Dec. of 1993.

M. Talebian, (research assistantship 50%, Oct. 1993 to Dec. 1993, May–June, 1996)

Selim Guncer (postdoctoral research fellow, Sept. 1, 1994 to Aug. 31, 1995)

U. Hohenester (research assistant, Feb. to Oct. 1994, no financial support)